Success Story

ATOMIC STRUCTURE MODELS PROVIDE LINK TO PREDICTIONS OF PROPERTIES OF MATERIALS

Images of Screw Dislocation Cores in Gold and Iridium

Gold — Experimental / Calculated

Iridium — Experimental / Calculated

Iso-charge density plot showing atomic locations around the core of a screw dislocation in Molybdenum
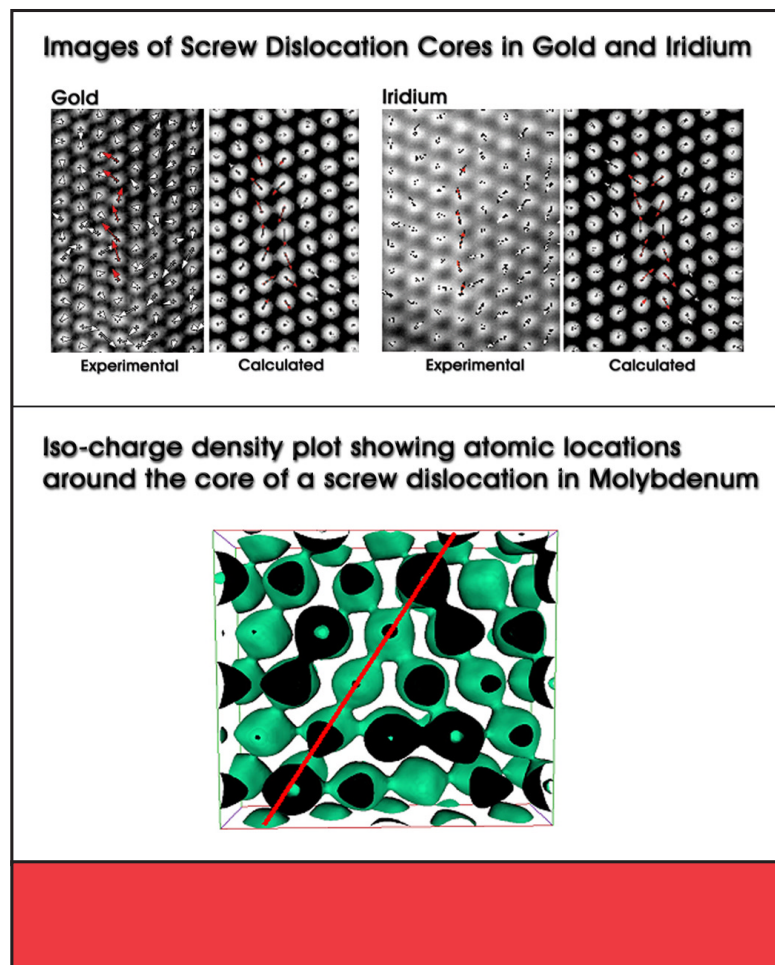
The Air Force Office of Scientific Research sponsored research to verify the accuracy of a model that predicts certain aspects of the deformation behavior of metals. This discovery will allow the Air Force to vastly decrease the scope, duration, and cost of testing materials used in weapon systems.

Accomplishment

Since 1998, the Metallic Materials program in the Aerospace and Materials Sciences Directorate funded two universities involved in the determination of atomic core structure of dislocations in various metals. First, Professor Arthur Freeman and his colleagues at Northwestern University, created a first-principles model that forecasts the atomic core structure of dislocations in gold and iridium.

Then, using high-resolution transmission electron microscopy, Professor Kevin Hemker and associates at Johns Hopkins University, achieved direct resolution of dislocation cores in gold and iridium. Professor Hemker's team proved that previous calculations by Professor Freeman's group accurately forecasted atomic positions around dislocation cores for several different dislocation configurations.

Background

Many useful engineering properties of materials depend on the type and distribution of defects in the arrangements of their atoms. Scientists rely on experiments to establish and validate materials, databases used in design, and selective use of computations, using physically based models to vastly decrease the scope, duration, and cost of experimental programs.

This computational strategy provides the foundation for programs leading to shorter design cycles that incorporate optimized techniques for materials selection and processing, resulting in more affordable and reliable weapon systems. Dislocations are the principal crystal defect responsible for permanent changes in the shape of crystalline materials.

Atomic models of dislocations, based on quantum mechanics, provide the necessary information to explain and predict differences in the deformation behavior of various metals. This information forms the basis for computational models that relate the behavior of a material to its thermo-mechanical environment, thus permitting computations of structure and property changes during processing and service.

Experimental verification of structures, based on models, increases confidence in the prediction of other properties that are more difficult to measure. Researchers at the Materials and Manufacturing Directorate developed a hybrid model that couples discrete and continuum descriptions of the crystal to calculate dislocation core structures in molybdenum.

Results of current research at Johns Hopkins will extend the capability for linking deformation behavior of these metals to their atomic structure. This will expand the capability for constructing accurate models for the design of materials and reduce costs of new materials.

Additional information